Full Band Simulation of Hole Transport in 1-D Heterostructures.

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As microelectronic research moves devices to nanometer scale operating at GHz speeds, the physics of electron flow through devices becomes more complicated and physical effects, which previously could be ignored safely in microelectronic devices, become significant. High energy electron injection, quantization of charge, quantization of energy, electron-electron, electron-photon and other electron scattering interactions are some of the phenomena that are presently being investigated experimentally and theoretically. Raytheon/TI developed a 1-D quantum device simulator (NEMO-1D) to address such issues. In 1-D heterostructures In that effort expertise in device physics, numerical and graphical user interface technologies were combined to produce the first quantitative, general-purpose quantum device simulator. The work presented here is an extension of the of the NEMO 1-D software to massively parallel high performance computing to enable the simulation of hole transport.

InSb-based inter band cascade lasers are good candidates for future far infrared lasers. They include the tunneling of hole into electron states. We started our study hole of transport in a simpler system where experimental data on hole transport is readily available: a hole resonant tunneling diode in GaAs/AlAs. Heterostructures such as resonant tunneling diodes break the symmetry of the crystalline lattice. Such break in lattice symmetry can cause a strong interaction of heavy-, light- and split-off hole bands. This strong interaction results in a complicated transverse subband dispersion.

Figure 1 shows transmission coefficients and transverse subband dispersions of two resonant tunneling structures: a GaAs/AlGaAs electron RTD and a GaAs/AlAs hole RTD. The RTD well and the barriers are 20 , 10 monolayers thick, respectively. The transverse momentum is normalized to the Brillouin zone. The transverse electron dispersion is almost parabolic and the transmission coefficient at transverse momentum of 0.039 appears to be a shifted version of the transmission at k=0.0. This is exactly the assumption used in the derivation of the Tsu-Esaki current formula. For holes, however, the dispersion shows a set of strongly interacting states. The dispersion is full characterized by several anti-crossings of light and heavy hole states. This strong interaction causes significant modulations in the transmission coefficient. The hole transmission coefficient at a transverse momentum of 0.039 has virtually no resemblance of the original transmission coefficient at 0.0 transverse momentum. The assumption underlying the Tsu-Esaki formula break down completely and the numerical integration over the transverse momentum becomes imperative.

Figure 1 indicates that the current flow is dominated by very sharp resonance linewidths (10^{-8} eV) in a large energy range that are non-local and sharply peaked in k-space. The integration in this space is computationally intensive since a multiband sp3s* second nearest neighbor model has to be used to reproduce the hole masses and anisotropies in the whole Brillouin zone properly. We have parallelized the integration over momentum and energy in the NEMO-1D code. This parallelization enabled the careful examination of the electron transport space. It was found that the current can be sharply spiked in k-space for k values that are outside the zone center at k=0. It is found that the dominant current contribution stems in wide bias ranges from holes that are traveling through the structure with non-zero transverse momentum (off the Γ zone center). The transverse subband dispersion causes the semiconductor to act like an indirect bandgap material for holes. Figure 2b indicates the current density J(k) at 4.2K that still needs to be integrated over the transverse momentum to obtain the final current density (Fig. 2a) as a function of bias. Significant current streaks outside the zone center resemble the transverse dispersion. Figure 2c shows a cut through J(k) at a bias of 0.2V. J(k) is sharply spiked on a linear as well as a logarithmic scale. Resolution of such spectral features is numerically daunting task.

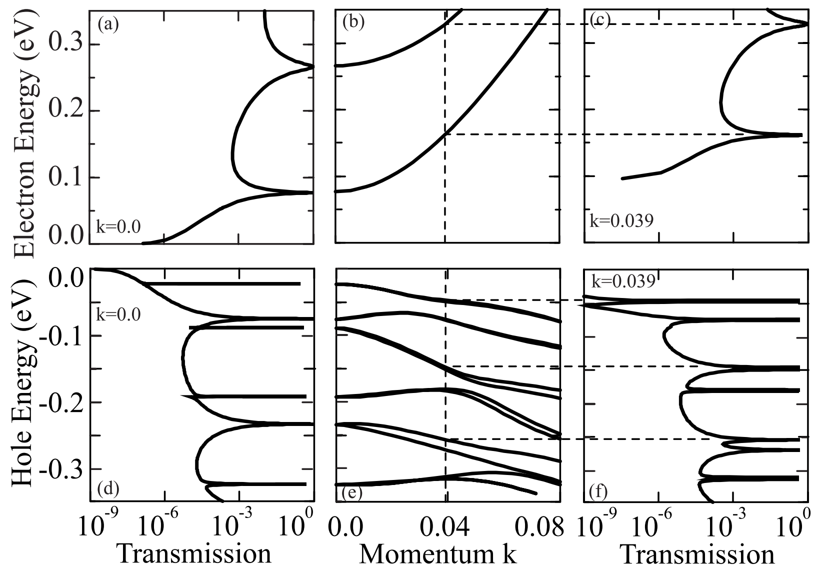

Figure 1: (a-c) Transmission coefficients and transverse dispersion of an electron RTD. (d-e) Equivalent figures for a hole RTD. Electron dispersion shows simple almost parabolic behavior while hole dispersion is exhibits strong band coupling and interactions between light and heavy holes. This strong interaction shows dramatic effects in the current voltage characteristic.

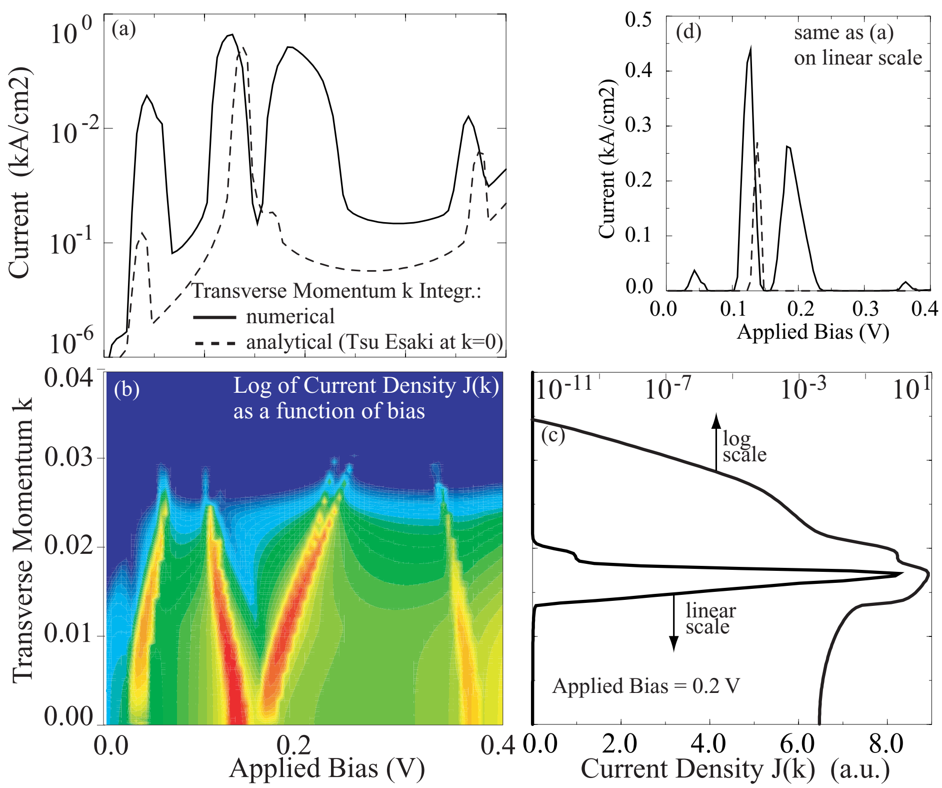

Figure 2: (a) Current-voltage characteristic of a hole resonant tunneling diode computed with and without explicit transverse momentum integration. Dashed curve corresponds to a cut through (b) at k=0. (b) Integrand current density J(k) as a function of transverse momentum and bias. Gray scale ranges from dark, over light back to dark. Almost vertical streaks indicate large current density along a pattern similar to the subband dispersion E(k) (c) Cut through (b) at a voltage of 0.2V on a linear and logarithmic scale. The most significant current contribution occurs at about k=0.018 off the zone center at k=0. (d) same as (a) on a linear scale. Full band integration in energy E and transverse momentum k is essential to capture all hole transport channels in a hole resonant tunneling diode.